

Benzylidene-p-isopropylphenylacetonitrile

Inchi: InChI=1S/C18H17N/c1-14(2)16-10-8-15(9-11-16)12-18(13-19)17-6-4-3-5-7-17/h3-12,14H
InchiKey: BLSSXJYYFIBNAQ-LDADJPATSA-N
Formula: C18H17N
SMILES: CC(C)c1ccc(C=C(C#N)c2ccccc2)cc1
Mol. weight [g/mol]: 247.33
CAS: 4452-07-7

Physical Properties

Property code	Value	Unit	Source
chs	-9746.00	kJ/mol	NIST Webbook
gf	518.28	kJ/mol	Joback Method
hf	313.77	kJ/mol	Joback Method
hfs	233.30	kJ/mol	NIST Webbook
hfus	26.94	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.874		Crippen Method
mcvol	214.040	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
tb	775.26	K	Joback Method
tc	1025.75	K	Joback Method
tf	388.93	K	Joback Method
vc	0.829	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.16	J/mol×K	775.26	Joback Method
cpg	599.47	J/mol×K	817.01	Joback Method
cpg	613.59	J/mol×K	858.76	Joback Method
cpg	626.62	J/mol×K	900.51	Joback Method
cpg	638.70	J/mol×K	942.25	Joback Method
cpg	649.93	J/mol×K	984.00	Joback Method
cpg	660.44	J/mol×K	1025.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4452077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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